

## Enabling Collaborative Combustion Data and Metadata Sharing

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In this poster we present a new informatics infrastructure designed to facilitate collaborative combustion science. Web-based data sharing for collaborative combustion research activities has become important in a growing number of projects. Two well-known examples in this community are the past work on GRI-Mech ([http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/)) and the Turbulent Nonpremixed Flame workshop series (<http://www.ca.sandia.gov/TNF/>). The new informatics infrastructure reported here is the first release from the Collaboratory for Multi-scale Chemical Science (CMCS, <http://cmcs.ca.sandia.gov/>). CMCS is implementing novel informatic data-sharing concepts, and is piloting this infrastructure among a multi-disciplinary team of chemical scientists working to advance combustion science.

The data infrastructure takes advantage of a variety of standards and open-source information technologies to provide an unprecedented ability to share data, data pedigree, and project information within groups and across communities. A shared data service provides configurable capabilities for automating the generation of metadata, translating data between standard formats, and federating multiple data stores. A portal serves as the web interface for the adaptable informatics infrastructure being developed by the CMCS team. The portal provides an array of functionality to support group and community processes, with an emphasis on simplifying the discovery and use of data. A pedigree browser can easily display pedigree data (as well as annotations) and allows users to search, browse, and retrieve a data set's pedigree. Pedigree data may also be an active link to a different, but associated, data resource.

To support the chemistry community, the CMCS team has integrated a variety of powerful chemistry applications, data viewers, and data translators. Examples of the implementation of the CMCS infrastructure in support of concepts and data in the context of experimental data and validations of combustion models are discussed. The capabilities that would support a collaborative data store for quantitative combustion diagnostics is also discussed.

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